CLAIMS

I claim:

1. In a method of calculating at least one physical parameter of a film in which the improvement comprising, the at least one physical parameter is related to scattering caused by interband states.

2. The method according to claim 1, wherein the at least one physical parameter is an optical property of the film.

3. The method according to claim 1, wherein the at least one physical parameter is selected from the group consisting of the optical dispersion, refractive index and the extinction coefficient of the film.

4. The method according to claim 1, wherein both the refractive index and the extinction coefficient of the film are calculated.

5. The method according to claim 1, wherein the at least one physical parameter is related to the scattering caused by interband states using a model.

6. The method according to claim 5, wherein the model includes a quantum mechanical transition equation for transitions between at least one of valence and conduction bands and interband states in a band gap.

7. The method according to claim 6, wherein the equation is:

$$\varepsilon_2(\omega) = \begin{cases} A\dfrac{\sqrt{E - E_D}}{E^2}, & \text{for } E > E_D \\ 0, & \text{for } E < E_D \end{cases}$$

where $\varepsilon_2(\omega)$ is the imaginary part of the dielectric function;

E is the incident photon energy;

E_D is the energy level of the interband state; and

wherein the values for A and E_D are fitted parameters obtained from measured data of an optical property of the film.

8. The method according to claim 7, wherein the model further includes the equation:

$$\varepsilon_1(\omega) = \begin{cases} \varepsilon_1(\infty) + A\dfrac{2\sqrt{E_D} - \sqrt{E_D+E} - \sqrt{E_D-E}}{E^2}, & \text{for } E < E_D \\ \varepsilon_1(\infty) + A\dfrac{2\sqrt{E_D} - \sqrt{E_D+E}}{E^2}, & \text{for } E > E_D \end{cases}$$

where $\varepsilon_1(\omega)$ is the real part of the dielectric function;

$\varepsilon_1(\infty)$ is the value of $\varepsilon_1(\omega)$ at infinite angular

frequency; and

wherein $\varepsilon_1(\infty)$ is a fitted parameter obtained from measured data of an optical property of the film.

9. The method according to claim 8, including using the values for $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ obtained by the modeling to calculate the physical parameters refractive index n and extinction coefficient *k* of the film according to the relations:

$$n = \sqrt{\frac{1}{2}\left[\sqrt{\left(\frac{\varepsilon_1}{\varepsilon_2}\right)^2 + \left(\frac{\varepsilon_2}{\varepsilon_0}\right)^2} + \frac{\varepsilon_2}{\varepsilon_0}\right]}$$

$$k = \sqrt{\frac{1}{2}\left[\sqrt{\left(\frac{\varepsilon_1}{\varepsilon_0}\right)^2 + \left(\frac{\varepsilon_2}{\varepsilon_0}\right)^2} + \frac{\varepsilon_1}{\varepsilon_0}\right]}$$

10. The method according to claim 7, wherein the measured data of an optical property of the film for obtaining the fitted parameters are from a reflectometer and/or an ellipsometer.

11. The method according to claim 1, wherein the film is a semiconductor material containing at least one alien species as an impurity forming interband states in the semiconductor material.

12. The method according to claim 1, wherein the film is selected from the group consisting of a semiconductor material and a dielectric material.

13. A method of material engineering for producing a film having at least one desired optical property by a process which alters interband states in the film to affect the property, comprising:

calibrating the magnitude of a process variable of the process to produce a film against a fitted parameter of a modeling equation for quantum mechanical transition between a band and interband states in a band gap in the film, which fitted parameter is a function of the magnitude of the process variable used to produce the processed film;

calculating the at least one optical property of a film for the corresponding value of the fitted parameter; and

deciding the magnitude of the process variable to be used in the process for producing a film having the desired at least one optical property.

14. The method according to claim 13, wherein the fitted parameter is A in the equation:

$$\varepsilon_2(\omega) = \begin{cases} A\dfrac{\sqrt{E - E_D}}{E^2}, & \text{for } E > E_D \\ 0, & \text{for } E < E_D \end{cases}$$

where $\varepsilon_2(\omega)$ is the imaginary part of the dielectric function;

E is the incident photon energy;

E_D is the energy level of the interband state; and

wherein the values for A and E_D are fitted parameters obtained from measured data of an optical property of the film.

15. The method according to claim 13, wherein the process variable is the rate of a gas flow containing an alien species used in the process.

16. The method according to claim 13, wherein the process variable is selected from the group consisting of the temperature and the time of processing the film.

17. The method according to claim 13, further comprising subjecting a film to the process which changes the concentration and/or level of interband states in the film; and monitoring the magnitude of the fitted parameter of the film produced by the process.

18. The method according to claim 13, wherein the film is a semiconductor or dielectric material.

19. In a process for producing a film having at least one desired optical property, wherein the process introduces or controls interband states in the film which affect the optical dispersion of the film, the improvement comprising:

calibrating the magnitude of a process variable used in the process to produce a film against a fitted parameter of a modeling equation for quantum mechanics transition between a band and interband states in a band gap in the film, which fitted parameter is a function of the magnitude of the process variable used to produce the film; and

monitoring the magnitude of the fitted parameter of the film produced by the process.

20. The process according to claim 19, wherein the fitted parameter is A in the equation:

$$\varepsilon_2(\omega) = \begin{cases} A\dfrac{\sqrt{E - E_D}}{E^2}, & \text{for } E > E_D \\ 0, & \text{for } E < E_D \end{cases}$$

where $\varepsilon_2(\omega)$ is the imaginary part of the dielectric function;

E is the incident photon energy;

E_D is the energy level of the interband state; and

wherein A and E_D are fitted parameters obtained from measured data of an optical property of the film.

21. The process according to claim 19, further comprising estimating the magnitude of the process variable used in the process from the monitored fitted parameter and the calibrating.

22. An apparatus for producing a film having at least one desired physical parameter, comprising:

a processing device for introducing or controlling interband states in a film which affect a physical parameter of the film;

an optical instrument for measuring a film which has been processed by the processing device, the optical instrument producing measured data as a result of the film measuring; and

a controller for adjusting the magnitude of a process variable of the processing by the processing device, the controller receiving the measured data from the optical instrument and having means for

calculating the physical parameter of the measured film using the measured data and a theoretical model relating the physical parameter to scattering caused by interband states in the film.

23. The apparatus according to claim 22, wherein the means for calculating is a programmed computer.

24. An apparatus comprising:

an optical instrument for measuring an optical property of a film containing interband states and producing measured data as a result of the film measuring; and

a programmed computer for calculating at least one physical parameter of the measured film using the measured data and a theoretical model relating the physical parameter to scattering caused by interband states.

25. The apparatus according to claim 24, wherein the optical instrument is selected from the group consisting of a reflectometer and an ellipsometer.